



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 01:28 PM UTC

PDB ID : 4R0M / pdb_00004r0m
Title : Structure of McyG A-PCP complexed with phenylalanyl-adenylate
Authors : Tan, X.F.; Dai, Y.N.; Zhou, K.; Jiang, Y.L.; Ren, Y.M.; Chen, Y.X.; Zhou, C.Z.
Deposited on : 2014-08-01
Resolution : 2.45 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

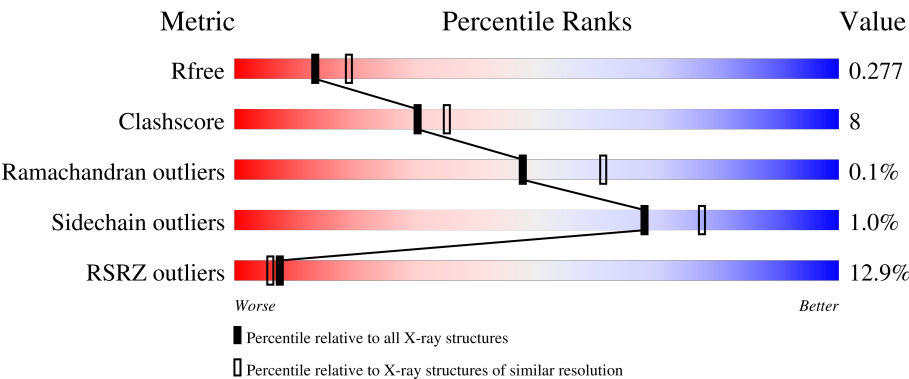
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.45 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1190 (2.46-2.46)
Clashscore	190562	1229 (2.46-2.46)
Ramachandran outliers	187476	1218 (2.46-2.46)
Sidechain outliers	187428	1218 (2.46-2.46)
RSRZ outliers	180081	1190 (2.46-2.46)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	643	12% 86% 12% ..
1	B	643	12% 76% 10% 14%

2 Entry composition [i](#)

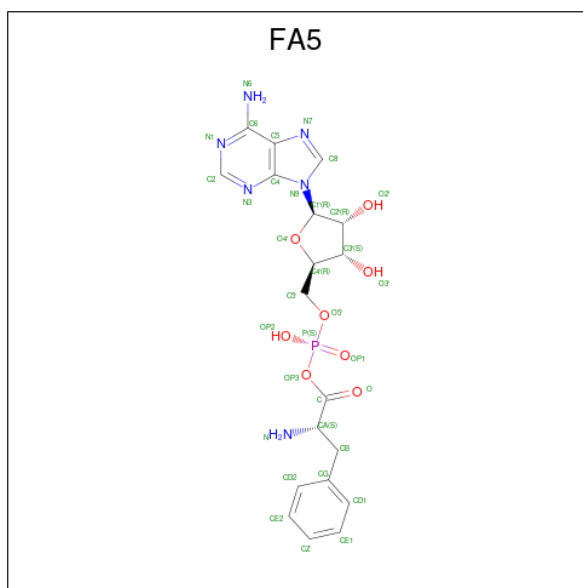
There are 3 unique types of molecules in this entry. The entry contains 9569 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called McyG protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	B	555	Total	C	N	O	S	Se	0	0	0
			4406	2824	736	835	3	8			
1	A	637	Total	C	N	O	S	Se	0	0	0
			5069	3242	854	961	3	9			

- Molecule 2 is ADENOSINE-5'-[PHENYLALANINYL-PHOSPHATE] (CCD ID: FA5) (formula: C₁₉H₂₃N₆O₈P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	N	O	P	0	0
			34	19	6	8	1		
2	A	1	Total	C	N	O	P	0	0
			34	19	6	8	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	16	Total	O	0	0
			16	16		
3	A	10	Total	O	0	0
			10	10		

4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	120.71Å 120.71Å 262.78Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	54.84 – 2.45 54.84 – 2.45	Depositor EDS
% Data completeness (in resolution range)	(Not available) (54.84-2.45) 98.5 (54.84-2.45)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.82 (at 2.45Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.247 , 0.273 0.248 , 0.277	Depositor DCC
R_{free} test set	4063 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	40.2	Xtriage
Anisotropy	0.183	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 20.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.019 for -h,-k,l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	9569	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.37% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FA5

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.67	2/5161 (0.0%)	0.81	7/6982 (0.1%)
1	B	0.64	0/4488	0.82	4/6074 (0.1%)
All	All	0.65	2/9649 (0.0%)	0.81	11/13056 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
All	All	0	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	479	THR	CA-C	-5.51	1.46	1.52
1	A	341	SER	C-O	-5.04	1.19	1.24

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	162	PRO	N-CA-C	-8.76	97.54	111.03
1	B	356	GLU	N-CA-C	-7.93	96.78	109.39
1	B	164	LYS	N-CA-C	-7.64	98.94	109.71
1	A	359	SER	N-CA-C	-7.63	98.14	110.20
1	A	478	GLU	CA-C-N	-7.37	112.60	122.99
1	A	478	GLU	C-N-CA	-7.37	112.60	122.99
1	A	341	SER	N-CA-C	6.12	117.62	108.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	480	ASP	N-CA-C	-5.75	101.76	110.28
1	A	519	ILE	N-CA-C	5.32	113.29	107.60
1	A	9	GLY	N-CA-C	5.20	125.51	113.18
1	B	519	ILE	N-CA-C	5.02	112.97	107.60

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	479	THR	Peptide
1	B	358	ASN	Peptide

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5069	0	5096	94	0
1	B	4406	0	4432	59	0
2	A	34	0	22	6	0
2	B	34	0	22	5	0
3	A	10	0	0	0	0
3	B	16	0	0	0	0
All	All	9569	0	9572	161	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (161) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:8:LEU:CD2	1:A:366:PRO:HD2	1.78	1.13
1:A:8:LEU:HD22	1:A:366:PRO:HD2	1.16	1.11
1:A:8:LEU:CD1	1:A:428:GLY:CA	2.36	1.04
1:B:355:THR:HB	1:B:357:GLU:HB2	1.40	1.01
1:A:313:ILE:HG21	1:A:349:LEU:CD1	1.90	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:8:LEU:HD22	1:A:366:PRO:CD	1.96	0.94
1:B:358:ASN:HB3	1:B:360:PHE:H	1.32	0.94
1:A:8:LEU:CD1	1:A:428:GLY:HA2	2.02	0.89
1:A:477:ARG:HB3	1:A:479:THR:OG1	1.71	0.89
1:A:8:LEU:CD1	1:A:428:GLY:HA3	2.04	0.87
2:B:701:FA5:HN1	2:B:701:FA5:H8	1.39	0.86
1:A:8:LEU:HD13	1:A:428:GLY:O	1.74	0.86
1:A:8:LEU:HD13	1:A:428:GLY:CA	2.06	0.85
1:B:358:ASN:CB	1:B:360:PHE:H	1.89	0.85
1:A:8:LEU:HD12	1:A:428:GLY:HA2	1.60	0.84
1:B:355:THR:O	1:B:357:GLU:N	2.13	0.81
1:A:475:GLN:O	1:A:477:ARG:N	2.13	0.81
1:B:298:MSE:HE1	1:B:300:PHE:C	2.06	0.80
1:B:60:ASN:ND2	1:B:163:SER:HA	1.97	0.79
1:B:353:GLU:O	1:B:357:GLU:HG2	1.82	0.78
1:B:355:THR:HG22	1:B:356:GLU:H	1.48	0.78
2:B:701:FA5:H8	2:B:701:FA5:N	1.99	0.77
1:A:334:PHE:CZ	1:A:336:MSE:HE3	2.21	0.76
2:A:701:FA5:HN2	2:A:701:FA5:HD1	1.49	0.76
1:A:8:LEU:HD13	1:A:428:GLY:C	2.11	0.76
1:A:8:LEU:HD12	1:A:428:GLY:CA	2.15	0.75
1:A:298:MSE:HE2	1:A:301:LEU:CA	2.18	0.74
1:B:298:MSE:HE2	1:B:301:LEU:HB2	1.72	0.71
1:A:313:ILE:HG21	1:A:349:LEU:HD11	1.71	0.71
1:B:355:THR:HG22	1:B:356:GLU:N	2.05	0.70
1:A:475:GLN:C	1:A:476:SER:HG	2.00	0.70
1:A:298:MSE:HE2	1:A:301:LEU:HA	1.73	0.70
1:B:226:HIS:HE1	2:B:701:FA5:HB1	1.55	0.70
1:B:313:ILE:HG21	1:B:349:LEU:HD13	1.74	0.69
1:A:298:MSE:CE	1:A:300:PHE:C	2.66	0.69
1:A:464:VAL:O	1:A:465:SER:OG	2.06	0.69
1:A:475:GLN:O	1:A:476:SER:OG	2.05	0.69
1:B:372:ILE:HG22	1:B:392:ILE:HG22	1.74	0.68
1:A:504:ARG:HH11	1:A:504:ARG:HG2	1.60	0.67
2:A:701:FA5:HN1	2:A:701:FA5:H8	1.59	0.67
1:A:468:ALA:HB3	1:A:485:THR:OG1	1.93	0.67
1:B:303:ASN:HD22	1:B:313:ILE:HD11	1.60	0.66
1:A:271:SER:H	1:A:298:MSE:HE1	1.59	0.66
1:A:350:SER:H	1:A:351:LYS:C	2.03	0.65
1:B:355:THR:H	1:B:357:GLU:HB3	1.59	0.65
1:A:8:LEU:CD2	1:A:366:PRO:CD	2.62	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:701:FA5:HD1	2:B:701:FA5:HN2	1.61	0.65
1:B:298:MSE:CE	1:B:300:PHE:H	2.10	0.64
1:B:351:LYS:O	1:B:351:LYS:HG2	1.97	0.64
1:B:355:THR:C	1:B:357:GLU:N	2.55	0.64
1:A:372:ILE:HG22	1:A:392:ILE:HG22	1.77	0.64
1:A:298:MSE:HE2	1:A:300:PHE:C	2.23	0.64
1:A:298:MSE:HE2	1:A:301:LEU:N	2.12	0.64
1:A:226:HIS:HE1	2:A:701:FA5:HB1	1.63	0.63
1:B:355:THR:CB	1:B:357:GLU:HB2	2.24	0.62
1:A:313:ILE:CG2	1:A:349:LEU:CD1	2.75	0.62
1:A:334:PHE:CZ	1:A:336:MSE:CE	2.83	0.61
1:A:6:ILE:O	1:A:6:ILE:HG23	2.00	0.61
1:A:352:ASN:OD1	1:A:352:ASN:O	2.18	0.61
1:A:350:SER:H	1:A:351:LYS:CA	2.15	0.60
1:A:202:MSE:HE1	1:A:236:MSE:CE	2.31	0.60
1:B:357:GLU:O	1:B:359:SER:HA	2.01	0.60
1:B:298:MSE:CE	1:B:300:PHE:N	2.65	0.59
1:A:250:GLU:H	1:A:250:GLU:CD	2.10	0.59
1:A:468:ALA:HB3	1:A:485:THR:HG1	1.67	0.59
1:A:8:LEU:HD11	1:A:428:GLY:HA3	1.85	0.58
1:B:64:GLN:HE22	1:B:162:PRO:HG2	1.69	0.58
1:A:475:GLN:N	1:A:475:GLN:OE1	2.38	0.57
1:A:352:ASN:OD1	1:A:356:GLU:OE2	2.23	0.56
1:A:271:SER:N	1:A:298:MSE:HE1	2.19	0.56
1:B:298:MSE:HE3	1:B:299:LYS:N	2.20	0.56
1:A:611:GLN:HE22	1:A:624:LEU:HD23	1.70	0.56
1:A:298:MSE:HE3	1:A:300:PHE:H	1.71	0.55
1:A:356:GLU:O	1:A:357:GLU:HB3	2.05	0.55
1:B:484:ILE:HD12	1:B:515:PRO:HB3	1.88	0.55
1:B:508:THR:HG22	1:B:514:ALA:HB2	1.89	0.55
1:B:298:MSE:CE	1:B:300:PHE:C	2.78	0.55
1:A:350:SER:N	1:A:351:LYS:HA	2.22	0.55
1:B:494:GLU:HB3	1:B:497:ILE:HD11	1.88	0.54
1:A:275:ASN:ND2	1:A:309:SER:H	2.06	0.54
2:A:701:FA5:HD1	2:A:701:FA5:N	2.22	0.53
1:A:350:SER:N	1:A:351:LYS:CA	2.71	0.53
1:B:298:MSE:HE3	1:B:300:PHE:H	1.73	0.53
1:B:298:MSE:HE1	1:B:300:PHE:H	1.73	0.53
1:A:14:ASP:OD1	1:A:197:HIS:HE1	1.92	0.53
1:B:190:LYS:HD2	1:B:407:LEU:HD21	1.91	0.53
1:B:545:GLN:N	1:B:546:GLY:HA2	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:351:LYS:HA	1:B:354:LEU:HD12	1.91	0.53
1:B:493:PHE:HA	1:B:495:GLN:H	1.74	0.53
1:B:75:LEU:HB2	1:B:99:PRO:HA	1.91	0.52
1:B:60:ASN:HD22	1:B:163:SER:HA	1.73	0.52
1:A:335:GLY:O	2:A:701:FA5:N	2.43	0.52
1:A:350:SER:H	1:A:351:LYS:HA	1.75	0.51
1:A:8:LEU:HD13	1:A:428:GLY:HA2	1.77	0.51
1:B:464:VAL:O	1:B:465:SER:OG	2.24	0.51
1:A:350:SER:HB2	1:A:354:LEU:HB2	1.93	0.51
1:B:353:GLU:O	1:B:357:GLU:CG	2.55	0.50
1:A:350:SER:OG	1:A:353:GLU:N	2.44	0.50
1:B:298:MSE:HE3	1:B:300:PHE:N	2.27	0.50
1:B:508:THR:CG2	1:B:514:ALA:HB2	2.41	0.50
1:B:72:LYS:HD2	1:B:123:LEU:HD22	1.94	0.49
1:B:213:THR:O	1:B:216:GLU:HG2	2.12	0.49
1:B:541:LYS:O	1:B:545:GLN:HG2	2.13	0.49
1:A:478:GLU:O	1:A:478:GLU:HG3	2.12	0.49
1:A:357:GLU:O	1:A:357:GLU:CD	2.55	0.48
1:A:334:PHE:HZ	1:A:336:MSE:CE	2.27	0.48
1:A:313:ILE:HG21	1:A:349:LEU:HD13	1.88	0.47
1:B:298:MSE:HE1	1:B:300:PHE:N	2.29	0.47
1:A:270:ILE:HA	1:A:298:MSE:HE1	1.95	0.47
1:A:376:ASP:HB3	1:A:382:LEU:HD21	1.96	0.47
1:A:313:ILE:HG21	1:A:349:LEU:HD12	1.88	0.47
1:A:334:PHE:CE2	1:A:336:MSE:HE3	2.49	0.46
1:A:475:GLN:N	1:A:475:GLN:CD	2.73	0.46
1:A:72:LYS:HD3	1:A:123:LEU:HD22	1.98	0.46
1:A:336:MSE:HE2	1:A:336:MSE:HB3	1.81	0.46
1:A:6:ILE:CG1	1:A:425:LEU:HB2	2.46	0.46
1:A:202:MSE:HE1	1:A:236:MSE:HE3	1.97	0.46
1:B:351:LYS:O	1:B:351:LYS:CG	2.63	0.46
1:A:455:THR:HG22	1:A:506:HIS:HD2	1.81	0.46
1:B:272:TRP:HB2	1:B:302:VAL:HB	1.98	0.45
1:A:350:SER:HB2	1:A:354:LEU:CB	2.47	0.45
1:A:474:ASP:CG	1:A:475:GLN:N	2.74	0.45
1:A:6:ILE:HD12	1:A:384:GLU:HA	1.99	0.45
1:B:199:ILE:O	1:B:203:THR:HG23	2.17	0.45
1:B:298:MSE:HE2	1:B:301:LEU:N	2.32	0.45
1:A:420:GLY:O	1:A:435:ARG:HG3	2.17	0.45
1:A:135:ILE:O	1:A:139:GLU:HG3	2.16	0.45
2:A:701:FA5:H8	2:A:701:FA5:N	2.30	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:376:ASP:HB3	1:B:382:LEU:HD21	1.98	0.45
1:A:477:ARG:HD2	1:A:479:THR:OG1	2.17	0.45
1:B:500:VAL:HG13	1:B:518:VAL:HB	1.98	0.45
1:A:206:THR:HG21	1:A:236:MSE:HE1	1.97	0.45
1:A:194:LEU:HD22	1:A:340:CYS:SG	2.57	0.45
1:B:142:GLY:HA3	1:B:150:TRP:CD1	2.52	0.44
1:B:317:LEU:HG	1:B:330:ILE:HD12	1.99	0.44
1:A:298:MSE:CE	1:A:300:PHE:O	2.65	0.44
1:A:482:LEU:HD22	1:A:513:ILE:HD12	1.99	0.44
1:A:199:ILE:HG23	1:A:231:VAL:HG13	2.00	0.44
1:A:334:PHE:HZ	1:A:336:MSE:HE1	1.83	0.44
1:B:358:ASN:HB2	1:B:360:PHE:H	1.77	0.43
1:A:8:LEU:HD23	1:A:366:PRO:CG	2.49	0.43
1:A:36:TYR:HE1	1:A:84:ILE:HD12	1.84	0.43
1:A:475:GLN:C	1:A:477:ARG:N	2.73	0.43
1:A:487:SER:HA	1:A:488:PRO:HD3	1.90	0.43
1:A:313:ILE:CG2	1:A:349:LEU:HD12	2.48	0.42
1:A:298:MSE:HE3	1:A:300:PHE:C	2.42	0.42
2:B:701:FA5:N	2:B:701:FA5:HD1	2.31	0.42
1:B:199:ILE:HG23	1:B:231:VAL:HG13	2.00	0.42
1:A:331:LYS:HD2	1:A:346:SER:O	2.20	0.42
1:B:36:TYR:HE1	1:B:84:ILE:HD12	1.84	0.41
1:B:522:GLU:CD	1:B:522:GLU:H	2.28	0.41
1:A:142:GLY:HA3	1:A:150:TRP:CD1	2.56	0.41
1:B:556:ASP:HA	1:B:559:LEU:HD12	2.03	0.41
1:B:298:MSE:CE	1:B:301:LEU:N	2.83	0.41
1:B:313:ILE:HG21	1:B:349:LEU:CD1	2.49	0.41
1:A:202:MSE:SE	1:A:202:MSE:C	3.14	0.41
1:A:504:ARG:HH11	1:A:504:ARG:CG	2.32	0.41
1:A:90:CYS:HB3	1:A:95:ILE:O	2.21	0.41
1:A:202:MSE:HE1	1:A:236:MSE:HE1	2.00	0.40
1:A:36:TYR:HD1	1:A:80:ASN:HB3	1.87	0.40
1:B:390:LEU:HD22	1:B:432:ILE:HD11	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	635/643 (99%)	618 (97%)	16 (2%)	1 (0%)	43	54
1	B	553/643 (86%)	537 (97%)	16 (3%)	0	100	100
All	All	1188/1286 (92%)	1155 (97%)	32 (3%)	1 (0%)	48	61

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	6	ILE

5.3.2 Protein sidechains

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	564/560 (101%)	556 (99%)	8 (1%)	59	72
1	B	490/560 (88%)	487 (99%)	3 (1%)	78	86
All	All	1054/1120 (94%)	1043 (99%)	11 (1%)	68	77

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	8	LEU
1	B	287	GLU
1	B	522	GLU
1	A	7	SER
1	A	247	VAL

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Mol	Chain	Res	Type
1	A	250	GLU
1	A	287	GLU
1	A	353	GLU
1	A	475	GLN
1	A	479	THR
1	A	484	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	15	ASN
1	B	39	ASN
1	B	60	ASN
1	B	76	GLN
1	B	146	HIS
1	B	156	ASN
1	B	226	HIS
1	B	255	GLN
1	B	267	GLN
1	B	294	ASN
1	B	326	GLN
1	B	358	ASN
1	B	438	GLN
1	A	30	ASN
1	A	76	GLN
1	A	81	GLN
1	A	125	ASN
1	A	197	HIS
1	A	226	HIS
1	A	258	GLN
1	A	267	GLN
1	A	275	ASN
1	A	290	HIS
1	A	326	GLN
1	A	352	ASN
1	A	443	ASN
1	A	492	GLN
1	A	506	HIS
1	A	567	GLN
1	A	611	GLN
1	A	612	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
2	FA5	B	701	-	36,37,37	1.31	4 (11%)	50,54,54	1.71	9 (18%)
2	FA5	A	701	-	36,37,37	1.31	4 (11%)	50,54,54	1.69	10 (20%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FA5	B	701	-	-	3/21/39/39	0/4/4/4
2	FA5	A	701	-	-	6/21/39/39	0/4/4/4

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	701	FA5	C5-C4	4.90	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	701	FA5	C5-C4	4.86	1.47	1.39
2	A	701	FA5	C5-C6	2.87	1.49	1.41
2	B	701	FA5	C5-C6	2.84	1.48	1.41
2	A	701	FA5	C8-N7	2.28	1.36	1.31
2	B	701	FA5	C5-N7	-2.27	1.34	1.39
2	B	701	FA5	C8-N7	2.26	1.36	1.31
2	A	701	FA5	C5-N7	-2.20	1.35	1.39

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	701	FA5	C5-C4-N3	-5.83	118.69	126.72
2	A	701	FA5	C5-C4-N3	-5.54	119.09	126.72
2	B	701	FA5	N3-C4-N9	4.59	134.97	127.17
2	A	701	FA5	N3-C4-N9	4.40	134.66	127.17
2	A	701	FA5	C2-N3-C4	3.78	121.07	111.83
2	B	701	FA5	C2-N3-C4	3.77	121.03	111.83
2	A	701	FA5	N3-C2-N1	-3.52	123.25	128.58
2	B	701	FA5	C4-C5-N7	-3.47	106.61	110.58
2	B	701	FA5	N3-C2-N1	-3.32	123.55	128.58
2	A	701	FA5	C4-C5-N7	-3.31	106.79	110.58
2	B	701	FA5	C5-N7-C8	2.45	107.30	103.45
2	B	701	FA5	CG-CB-CA	2.44	119.13	114.13
2	A	701	FA5	C4-N9-C8	2.42	108.27	105.74
2	A	701	FA5	C5-N7-C8	2.37	107.17	103.45
2	A	701	FA5	CG-CB-CA	2.34	118.92	114.13
2	B	701	FA5	C4-N9-C8	2.28	108.14	105.74
2	A	701	FA5	C6-C5-N7	2.26	136.44	132.09
2	A	701	FA5	C-CA-N	-2.25	104.04	110.82
2	B	701	FA5	C6-C5-N7	2.19	136.31	132.09

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	701	FA5	C-OP3-P-O5'
2	B	701	FA5	CA-CB-CG-CD2
2	B	701	FA5	CA-CB-CG-CD1
2	A	701	FA5	CA-CB-CG-CD1
2	A	701	FA5	CA-CB-CG-CD2
2	B	701	FA5	C-OP3-P-O5'
2	A	701	FA5	OP3-C-CA-CB

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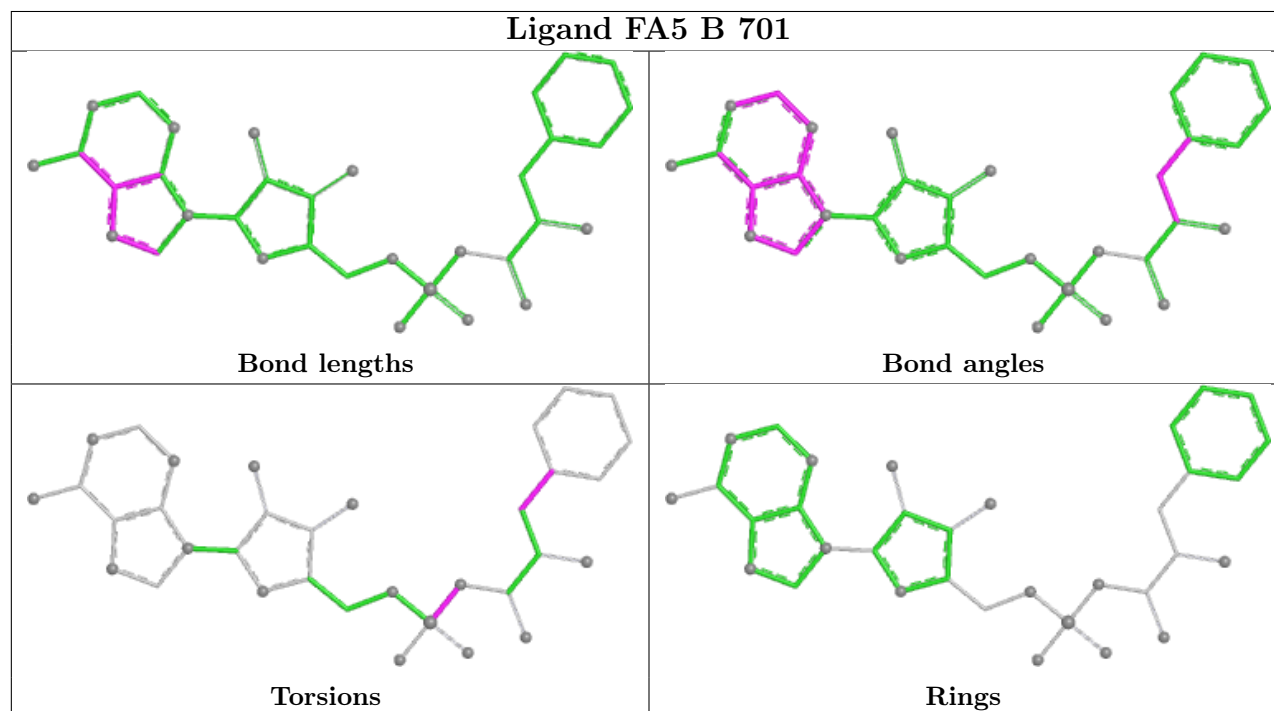
Mol	Chain	Res	Type	Atoms
2	A	701	FA5	O-C-CA-CB
2	A	701	FA5	C-OP3-P-OP1

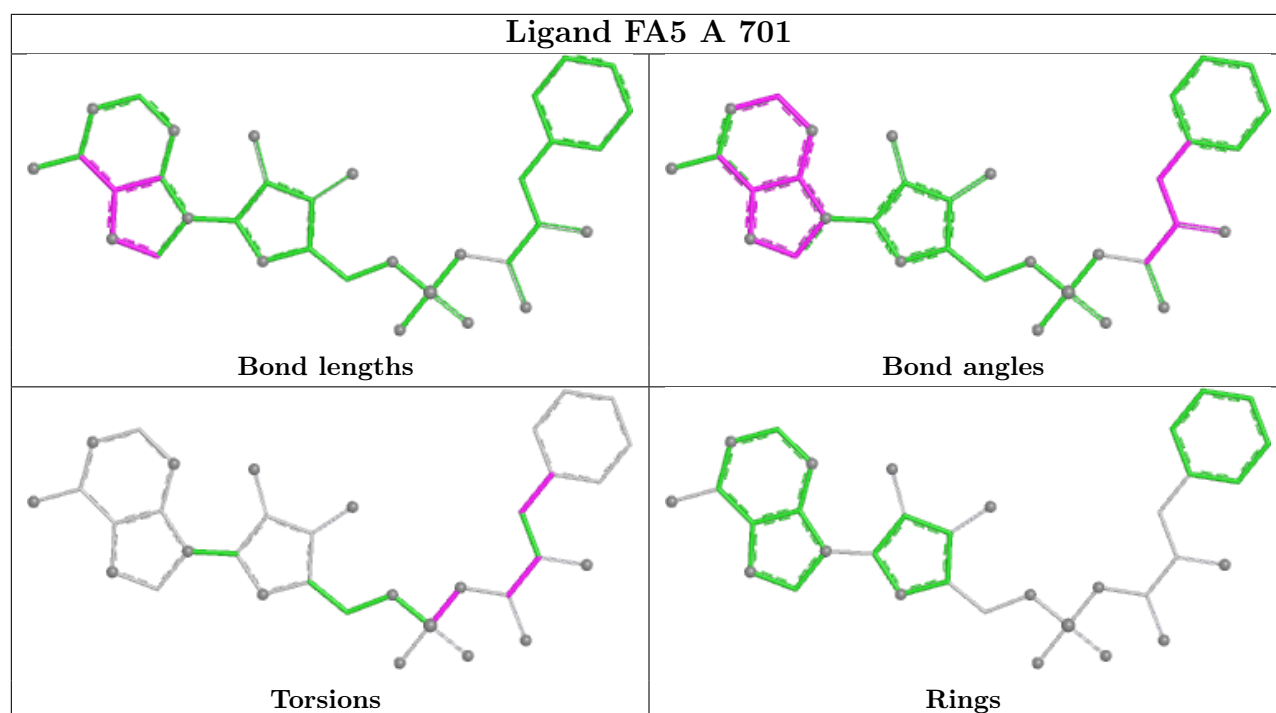
There are no ring outliers.

2 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	701	FA5	5	0
2	A	701	FA5	6	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	628/643 (97%)	0.78	77 (12%) 8 7	25, 41, 69, 99	1 (0%)
1	B	547/643 (85%)	0.79	74 (13%) 7 5	24, 40, 73, 104	0
All	All	1175/1286 (91%)	0.78	151 (12%) 7 6	24, 40, 70, 104	1 (0%)

All (151) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	8	LEU	7.8
1	B	493	PHE	7.8
1	B	165	ILE	7.4
1	A	351	LYS	7.2
1	B	8	LEU	7.1
1	A	624	LEU	7.1
1	A	354	LEU	7.0
1	B	164	LYS	6.6
1	A	358	ASN	6.4
1	A	9	GLY	5.9
1	A	479	THR	5.7
1	B	9	GLY	5.7
1	A	184	GLY	5.7
1	B	7	SER	5.7
1	B	494	GLU	5.6
1	A	185	SER	5.2
1	B	10	GLY	5.2
1	B	490	SER	5.2
1	B	561	LYS	5.1
1	B	497	ILE	5.1
1	A	352	ASN	5.0
1	A	359	SER	4.9
1	B	162	PRO	4.8
1	A	327	GLU	4.7

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Mol	Chain	Res	Type	RSRZ
1	B	560	ALA	4.7
1	B	31	ASN	4.6
1	A	5	SER	4.6
1	B	163	SER	4.5
1	B	350	SER	4.3
1	A	476	SER	4.2
1	A	186	THR	4.2
1	A	357	GLU	4.2
1	B	351	LYS	4.1
1	B	355	THR	4.1
1	B	358	ASN	4.1
1	A	478	GLU	4.0
1	B	166	GLU	4.0
1	A	475	GLN	3.9
1	A	10	GLY	3.9
1	B	491	GLU	3.9
1	B	496	GLY	3.8
1	B	542	ASP	3.8
1	B	359	SER	3.8
1	B	558	TYR	3.8
1	B	354	LEU	3.8
1	A	350	SER	3.7
1	A	356	GLU	3.6
1	B	498	LYS	3.6
1	A	6	ILE	3.4
1	B	357	GLU	3.4
1	A	616	LYS	3.4
1	A	355	THR	3.3
1	A	473	PHE	3.3
1	B	437	LYS	3.3
1	B	353	GLU	3.3
1	A	480	ASP	3.3
1	A	7	SER	3.3
1	B	187	GLY	3.3
1	B	499	VAL	3.2
1	B	161	ALA	3.1
1	B	183	SER	3.1
1	B	356	GLU	3.1
1	A	353	GLU	3.1
1	B	495	GLN	3.1
1	B	185	SER	3.0
1	B	30	ASN	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	545	GLN	3.0
1	A	524	ASN	3.0
1	B	508	THR	3.0
1	A	290	HIS	3.0
1	A	477	ARG	3.0
1	A	428	GLY	3.0
1	A	14	ASP	2.9
1	A	349	LEU	2.9
1	A	187	GLY	2.9
1	B	349	LEU	2.8
1	A	641	SER	2.8
1	A	640	LEU	2.8
1	B	381	PRO	2.8
1	B	186	THR	2.8
1	A	30	ASN	2.7
1	A	322	LYS	2.7
1	A	183	SER	2.7
1	A	639	PHE	2.6
1	A	550	SER	2.6
1	B	313	ILE	2.5
1	A	577	GLN	2.5
1	A	381	PRO	2.5
1	B	387	ILE	2.5
1	B	129	LEU	2.5
1	A	314	ARG	2.5
1	B	473	PHE	2.5
1	A	399	LYS	2.5
1	B	383	PRO	2.5
1	B	144	TYR	2.5
1	A	250	GLU	2.5
1	B	475	GLN	2.5
1	A	410	GLU	2.4
1	A	537	SER	2.4
1	A	623	SER	2.4
1	A	157	GLU	2.4
1	B	492	GLN	2.4
1	A	15	ASN	2.4
1	B	327	GLU	2.4
1	B	184	GLY	2.4
1	B	12	LEU	2.4
1	A	326	GLN	2.4
1	A	328	ARG	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	569	LEU	2.4
1	A	379	ASN	2.3
1	B	292	SER	2.3
1	B	555	ILE	2.3
1	B	543	PHE	2.3
1	B	133	GLU	2.3
1	A	11	GLN	2.3
1	A	604	SER	2.3
1	A	617	LEU	2.3
1	A	427	LYS	2.3
1	A	13	GLU	2.3
1	B	203	THR	2.2
1	A	485	THR	2.2
1	B	442	ILE	2.2
1	B	15	ASN	2.2
1	B	559	LEU	2.2
1	A	622	LEU	2.2
1	A	491	GLU	2.2
1	A	12	LEU	2.2
1	A	474	ASP	2.2
1	B	13	GLU	2.2
1	B	443	ASN	2.2
1	A	403	ASN	2.2
1	B	447	TYR	2.2
1	A	638	ARG	2.2
1	B	352	ASN	2.1
1	A	413	GLN	2.1
1	A	313	ILE	2.1
1	B	523	ARG	2.1
1	B	550	SER	2.1
1	A	310	VAL	2.1
1	B	386	GLU	2.1
1	B	450	HIS	2.1
1	A	472	VAL	2.1
1	A	619	ASN	2.1
1	B	554	GLU	2.1
1	B	290	HIS	2.1
1	A	625	ALA	2.1
1	B	314	ARG	2.1
1	A	385	ARG	2.1
1	A	564	GLN	2.0
1	B	29	HIS	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	44	TYR	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

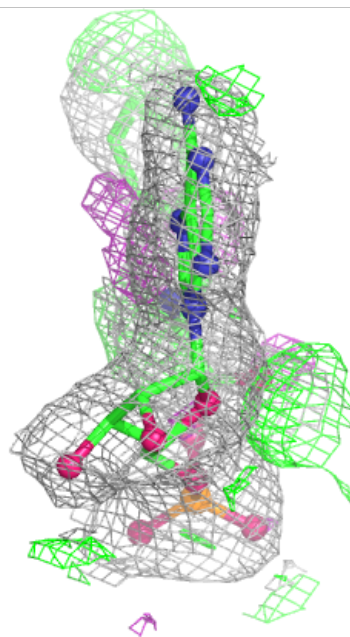
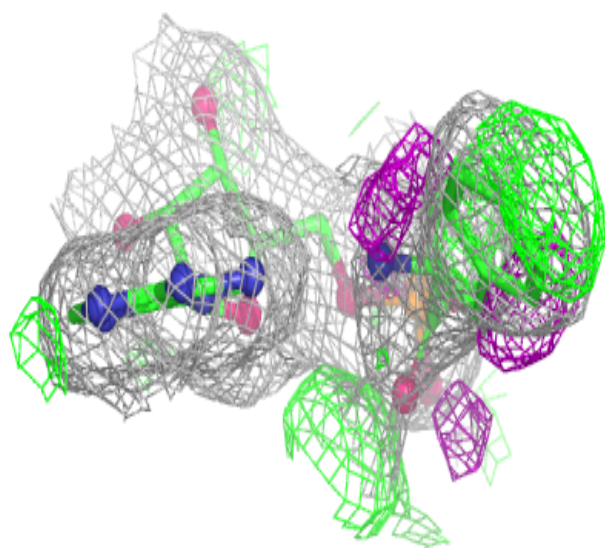
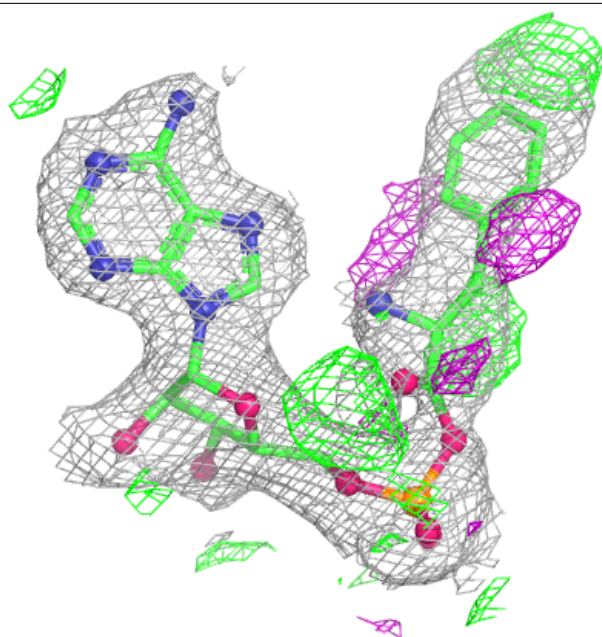
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	FA5	B	701	34/34	0.90	0.13	29,31,35,36	3
2	FA5	A	701	34/34	0.91	0.12	27,29,34,36	5

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

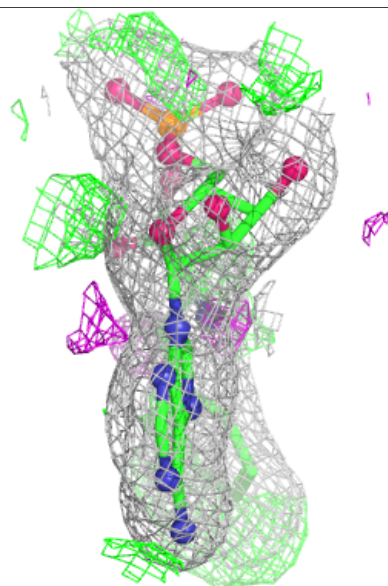
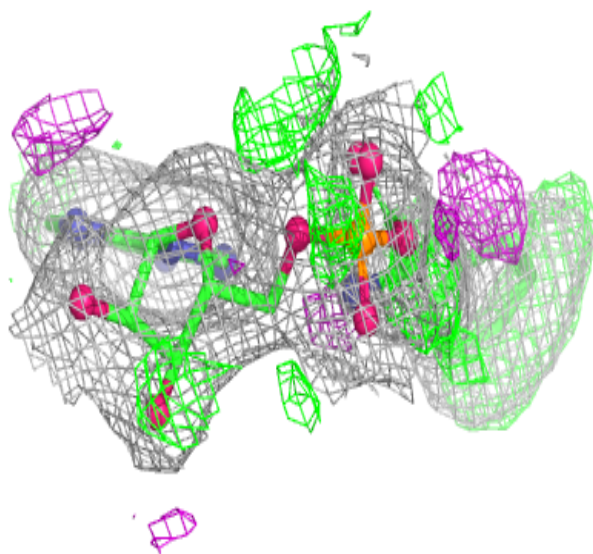
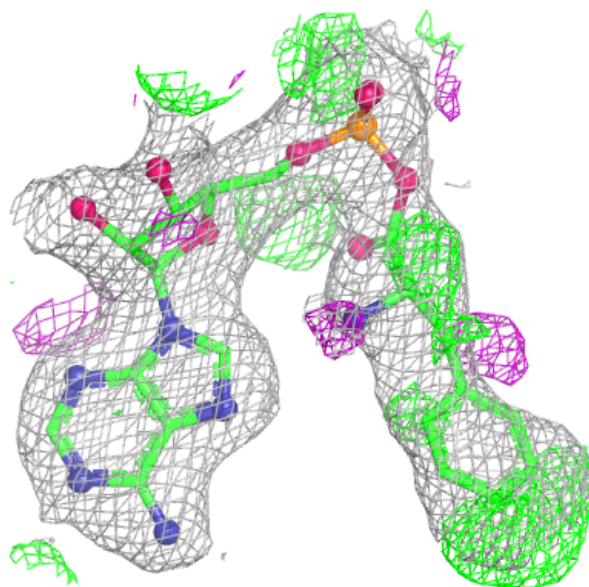
Electron density around FA5 B 701:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around FA5 A 701:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers ⓘ

There are no such residues in this entry.